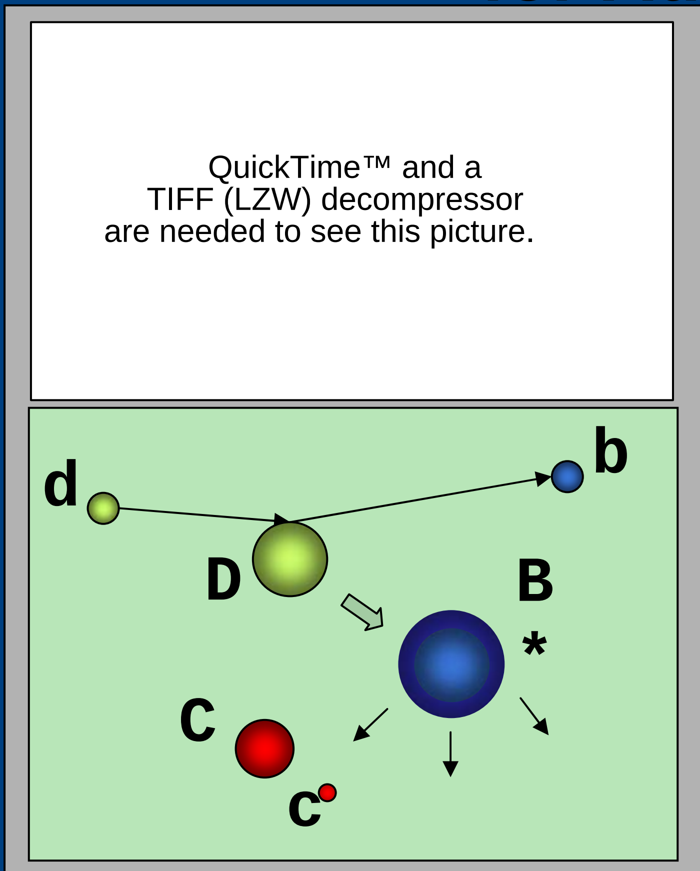
Surrogate Reactions for Advanced Fuel Cycles



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Lawrence Livermore National Lab

**Nuclear Physics and
Related Computational Science R&D for
Advanced Fuel Cycles
Workshop
Bethesda, MD, August 10-12, 2006**

This work is carried out under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48. Partial funding is provided by the LDRD program at LLNL.

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UCRL-PRES-xxxxxx

Physics & Advanced Technologies N Division

Outline

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II. Applications of the Surrogate approach

1. Applications in the Weisskopf-Ewing limit
2. Applications in the Ratio approximation
3. Using theory to test the assumptions underlying the analyses

III. Moving beyond current capabilities - R&D needs

1. Theory developments
2. Experimental developments

IV. Synopsis

I. The Surrogate idea

The Surrogate Nuclear Reactions approach is an indirect method for determining cross sections of compound-nuclear reactions that are difficult/impossible to measure directly.

Many reactions relevant to the AFC, to SBSS, and to astrophysics are compound-nuclear reactions. Often a direct measurement of the cross section is impractical or impossible.

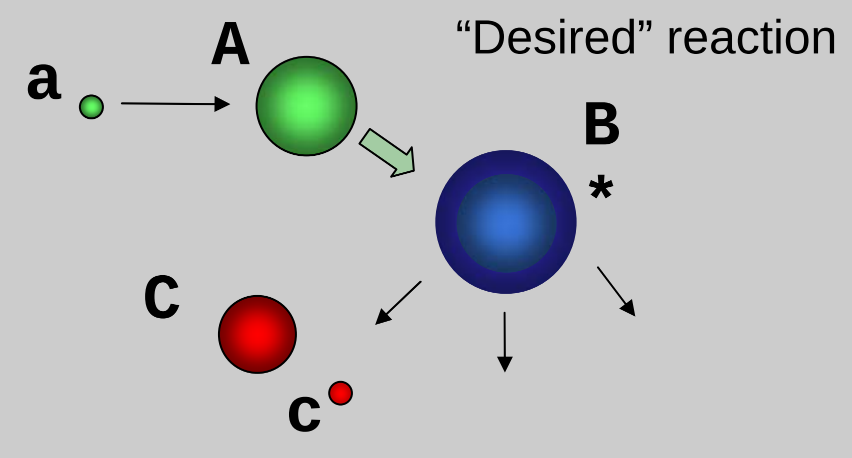
The Surrogate Idea

Hauser-Feshbach (HF) theory describes the "desired" compound-nuclear reaction

$$\sigma_{\alpha\chi} = \Sigma_{J,\pi}\, \sigma_\alpha^{CN}(E,J,\pi) \cdot G^{CN}_\chi(E,J,\pi)$$

The issue:

- the σ_α^{CN} can be calculated reasonably well
- the G^{CN}_χ are difficult to predict

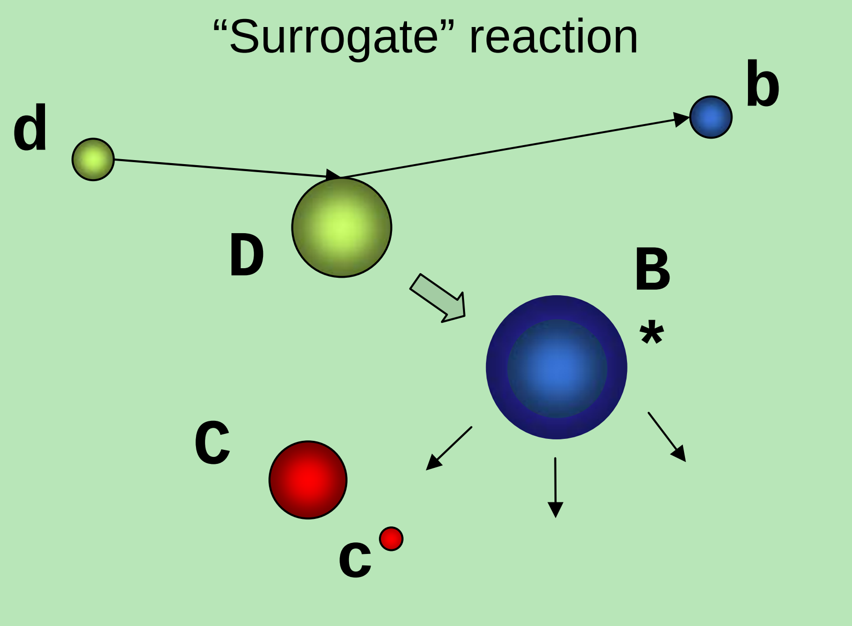


A Surrogate experiment provides

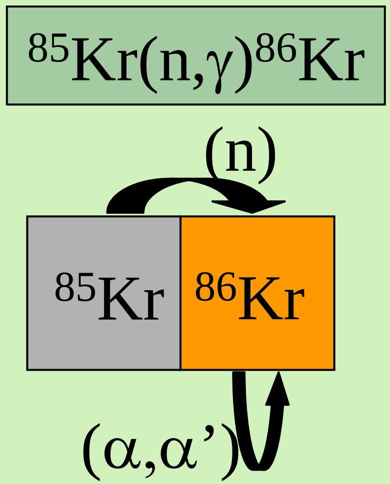
$$P_\chi(E) = \Sigma_{J,\pi}\, F_\delta^{CN}(E,J,\pi) \cdot G^{CN}_\chi(E,J,\pi)$$

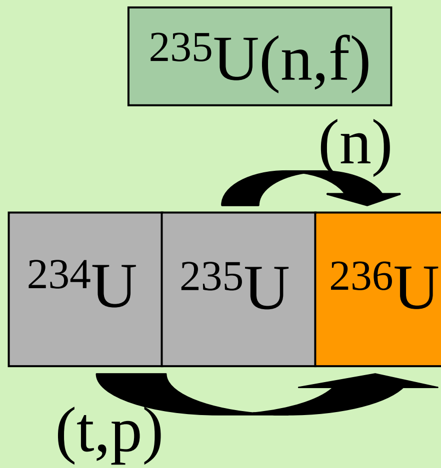
Procedure:

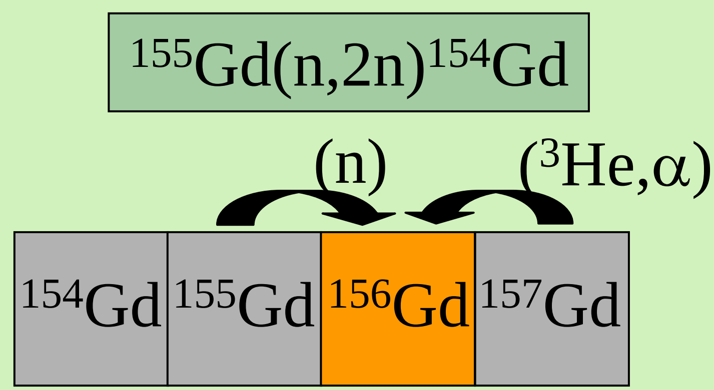
- calculate the direct-reaction probabilities $F_\delta^{CN}(E,J,\pi)$
- extract the decay probabilities $G^{CN}_\chi(E,J,\pi)$ and insert into the HF formula
- in practice: model the CN decay and obtain the G^{CN} by adjusting parameters in the HF calculation until the measured $P_\chi(E)$ are reproduced or *use approximations*



Surrogate reactions: some examples







The focus here is on neutron-induced reactions, although the Surrogate approach is more general.

II. Surrogate applications

In the past, almost all applications of the Surrogate method have relied on a simplifying assumption: the validity of the Weisskopf-Ewing limit. Two approaches have been used to analyze Surrogate experiments:

a) Surrogate reactions in the Weisskopf-Ewing limit (1970s and later)

b) Surrogate Ratio method (very recently)

The methods are usually verified *a posteriori* by comparing an extracted cross section with a direct measurements. This approach does not give enough information on the validity of the assumptions, the

The Weisskopf-Ewing limit

Hauser-Feshbach theory:

for the “desired” compound-nuclear reaction

$$\sigma_{\alpha\chi}(E) = \Sigma_{J,\pi}\, \sigma_{\alpha}^{CN}(E,J,\pi) \cdot G^{CN}_{\chi}(E,J,\pi)$$

Weisskopf-Ewing (WE) limit:

Decay probabilities are independent of J,π:

$$G^{CN}_{\chi}(E,J,\pi) \text{ ------> } G^{CN}_{\chi}(E)$$

Then:

$$\sigma_{\alpha\chi}^{WE}(E) = \sigma_{\alpha}^{CN}(E) \cdot G^{CN}_{\chi}(E)$$

where:

$$\sigma_{\alpha}^{CN}(E) = \Sigma_{J,\pi}\, \sigma_{\alpha}^{CN}(E,J,\pi)$$

Surrogate approach in the WE limit:

Decay probabilities independent of J,π implies:

$$P_{\chi}(E) = \Sigma_{J,\pi}\, F_{\delta}^{CN}(E,J,\pi) \cdot G^{CN}_{\chi}(E,J,\pi)$$

$$\text{------> } P_{\chi}(E) = G^{CN}_{\chi}(E)$$

since

$$\Sigma_{J,\pi}\, F_{\delta}^{CN}(E,J,\pi) = 1$$

and the deduced cross section for the desired reaction becomes simply:

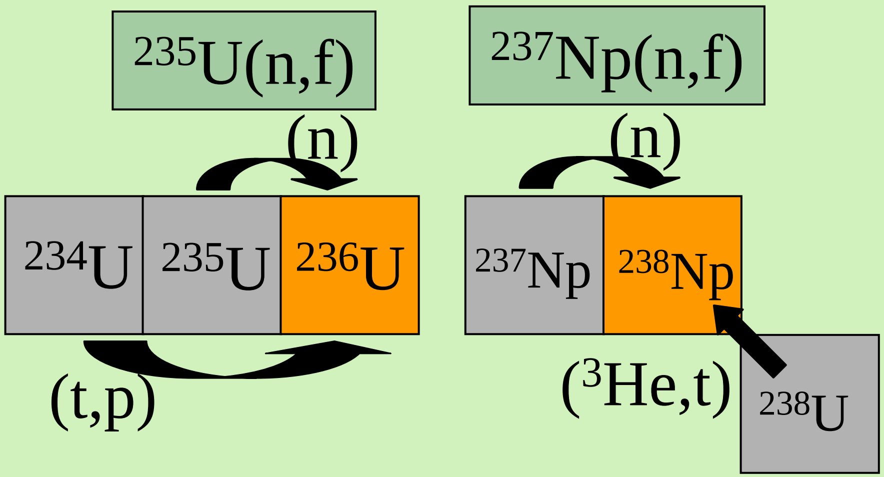
$$\sigma_{\alpha\chi}^{WE}(E) = \underbrace{\sigma_{\alpha}^{CN}(E)}_{\text{calculated}} \cdot \underbrace{P_{\chi}(E)}_{= N_{coinc}/N_{single} \text{ measured}}$$

Surrogate experiments analyzed in the WE approximation

Cramer and Britt, Nucl. Sci. Eng. **41** (1970) 177

Britt and Wilhelmy, Nucl. Sci. Eng. **72** (1979) 222

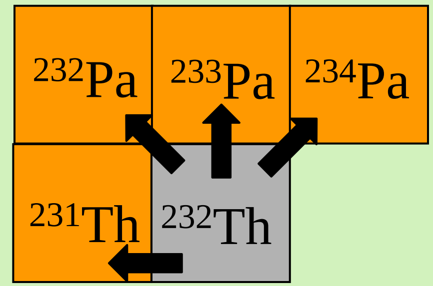
(n,f) cross section estimates for actinides based on Surrogate (t,p), (^{3}He,d) and (^{3}He,t) experiments



$\sigma_{(n,f)}(E) = \sigma^{CN}_{(n+A)}(E) \cdot P_f(E)$ with $P_f = N_{coinc}/N_{single}$

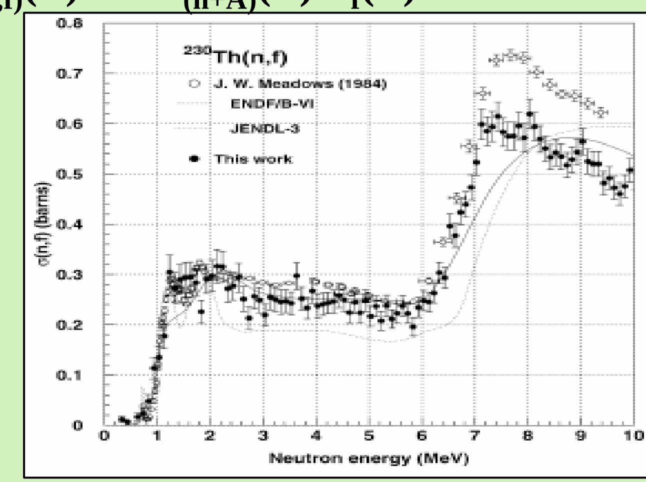
Petit et al., Nucl. Phys. A **735** (2004) 345

(n,f) cross sections for Th, Pa from Surrogate (^{3}He,x) experiments (x=α,t,d,p)



$\sigma_{(n,f)}$**(E)** is from a semi-microscopic optical-model

$\sigma_{(n,f)}(E) = \sigma^{CN}_{(n+A)}(E) \cdot P_f(E)$



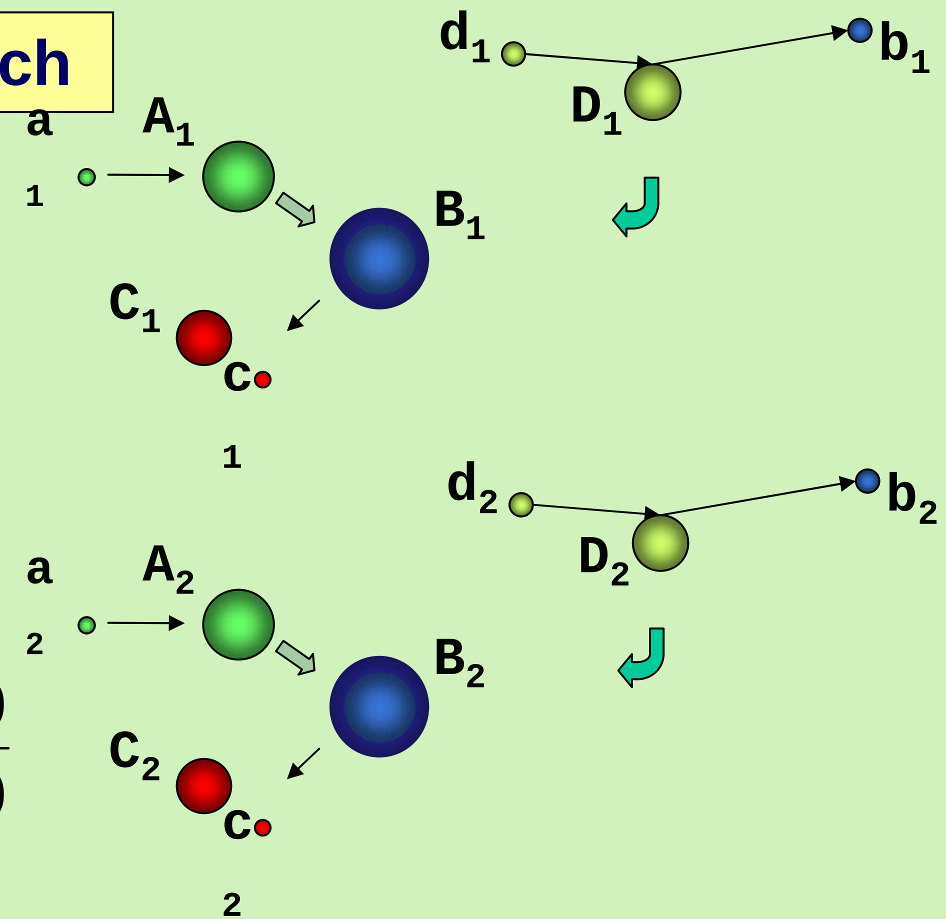
Approximations justified *a posteriori* by comparison with direct measurements.

The Surrogate Ratio approach

Goal: Determine experimentally

$$R(E) = \frac{\sigma_{\alpha_1 x_1}(E)}{\sigma_{\alpha_2 x_2}(E)}$$

and calculate the unknown cross section $\sigma_{\alpha_1 x_1}$
from the known cross section $\sigma_{\alpha_2 x_2}$



Procedure:

- Assume the validity of the WE limit:

$$R(E) \xrightarrow{\text{WE limit}} \frac{\sigma^{CN}_{\alpha_1}(E)}{\sigma^{CN}_{\alpha_2}(E)} \cdot \frac{G^{CN}_{\chi_1}(E)}{G^{CN}_{\chi_2}(E)}$$

- Use two Surrogate experiments to determine

$$\frac{G^{CN}_{\chi_1}(E)}{G^{CN}_{\chi_2}(E)} = \frac{N_{\text{coinc}}[\delta_1, \chi_1]}{N_{\text{coinc}}[\delta_2, \chi_2]} \cdot \underbrace{\frac{N_{\text{single}}[\delta_2]}{N_{\text{single}}[\delta_1]}}_{= \mathit{Norm}}$$

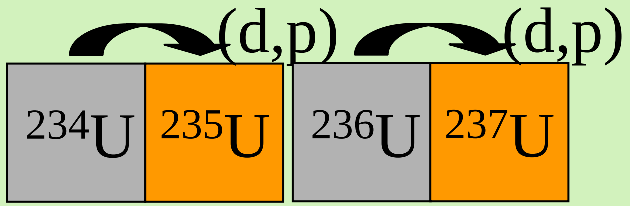
…where *Norm* accounts for differences in beam currents, target thicknesses, run times, etc. between the Surrogate experiments

Advantages of the Ratio approach:

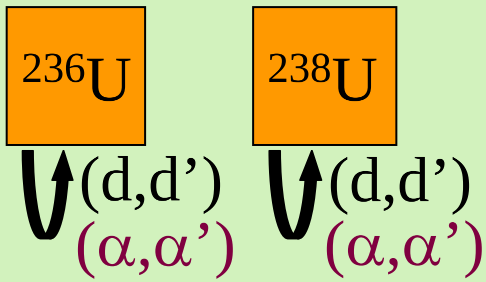
- Eliminates need to measure direct-reaction events
- Small systematic errors or violations of assumptions underlying a Surrogate WE analysis might cancel

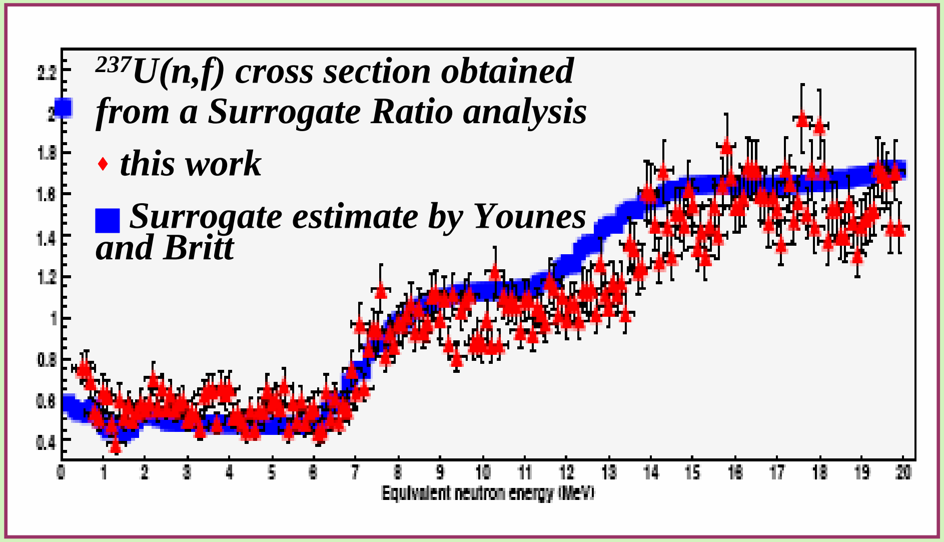
First results from the Surrogate Ratio approach

Plettner et al., PRC 71 (2005) 051602:



- (d,pf) on ^{238}U and ^{236}U to determine $\sigma[^{238}U(n,f)]/\sigma[^{236}U(n,f)]$
- (d,d'f) on ^{238}U and ^{236}U to determine $\sigma[^{237}U(n,f)]/\sigma[^{235}U(n,f)]$



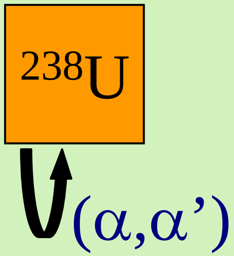


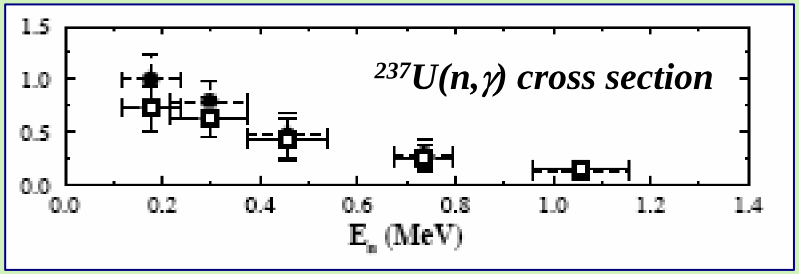
Burke et al., PRC 73 (2006) 054604:

- (α,α'f) on ^{238}U and ^{236}U to determine $\sigma[^{237}U(n,f)]/\sigma[^{235}U(n,f)]$

Bernstein et al., submitted (2006):

- (α,α'x) on ^{238}U, with x=f,γ,2n, to determine $\sigma[^{237}U(n,\gamma)]$ and $\sigma[^{237}U(n,2n)]$





Testing the assumptions underlying the analyses

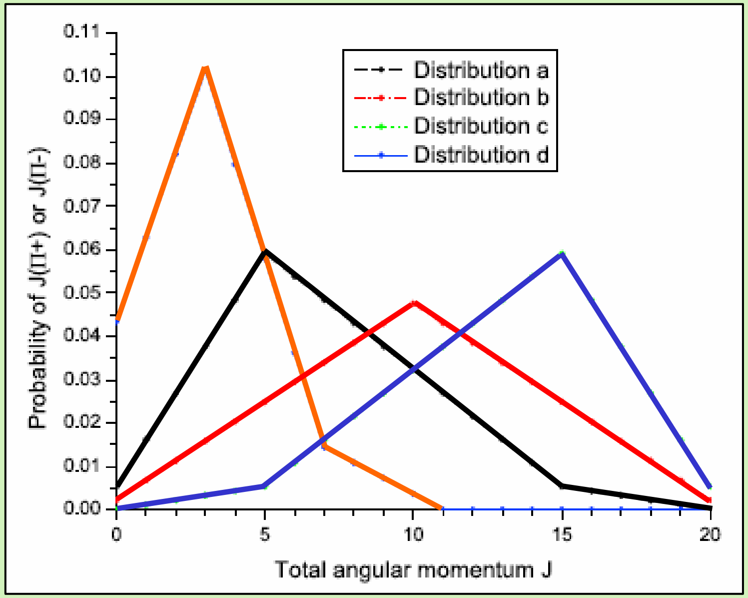
Theoretical study to address the following:

- Are the decay probabilities independent of spin and parity?
- Does a Surrogate analysis in the WE approximation yield reliable results?
- Does a Ratio analysis yield reliable results?

J. Escher and F.S. Dietrich
LLNL UCRL-JRNL-221555
(submitted)

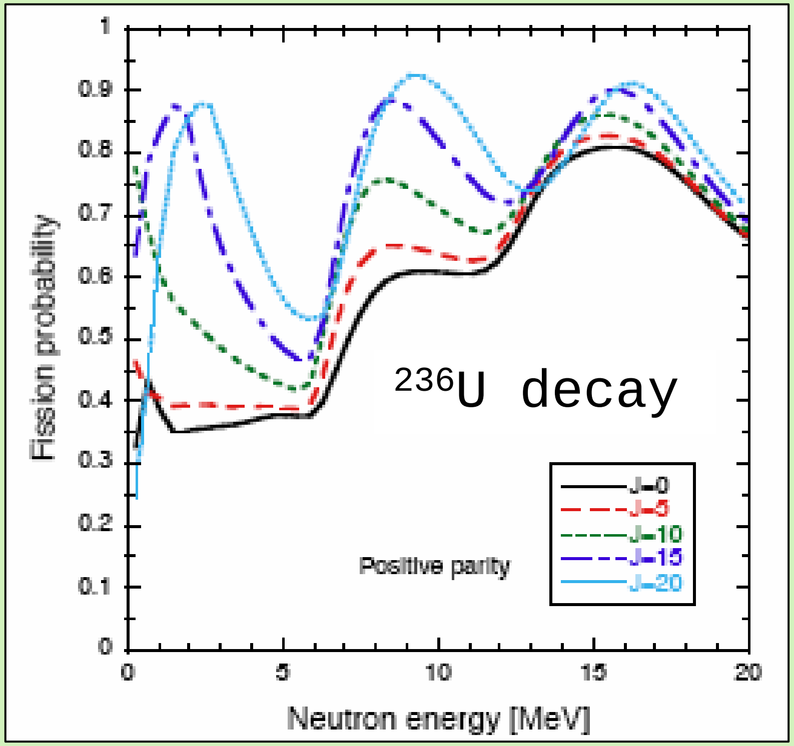
Simulation procedure:

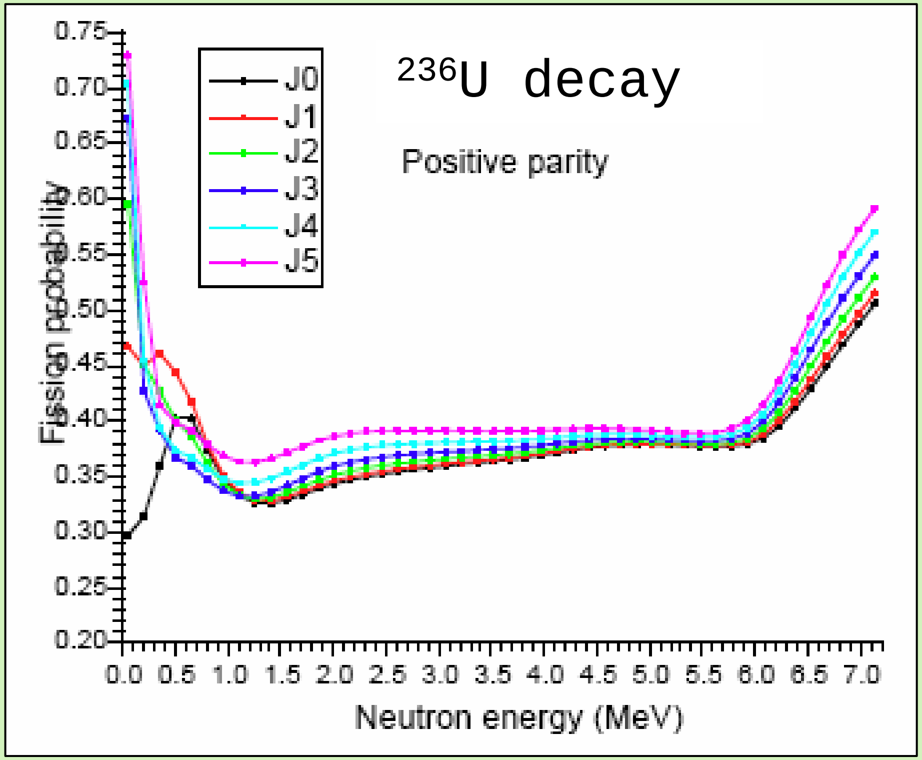
1. Determine "reference cross sections" with a statistical-model calculation ("benchmark").
2. Extract fission probabilities for each (J,π) and study as function of E_n.
3. Simulate a Surrogate experiment and carry out an analysis in the WE limit.
   Need to assume a J^π population for the CN.
4. Simulate two Surrogate experiments and carry out a Ratio analysis.
   Need to assume J^π populations for CN.



J^π distributions considered here

^{236}U fission probabilities for various J^π values



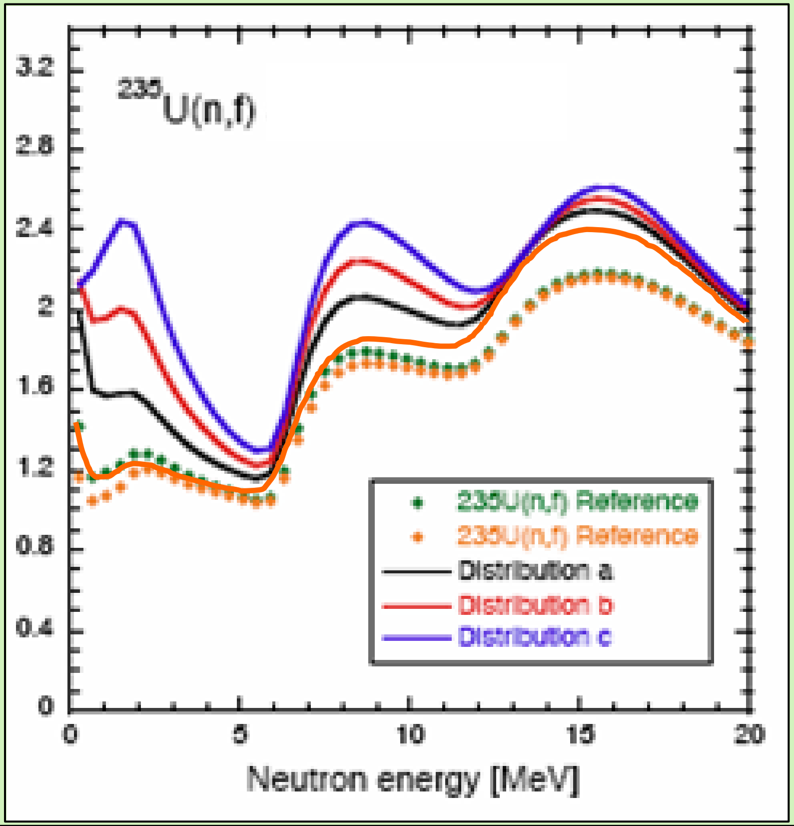


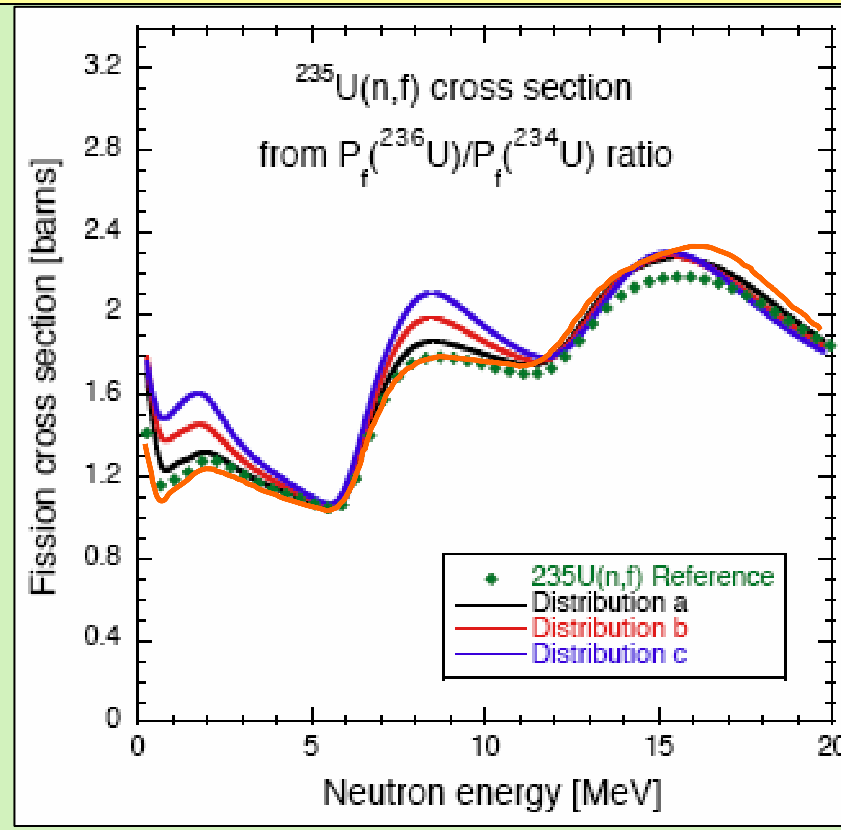
Observations:

- Fission probabilities show significant J^π dependence
- For small energies (E_n < 2 MeV) the WE approx is not valid
- Differences between fission probabilities increase at onset of 2nd chance fission
- Results depend little on parity (not shown)

It is not *a priori* obvious whether the WE limit applies to a particular reaction in a given energy regime. The validity of the WE approximation depends on the relevant J^π and E values.

(n,f) cross sections from our simulation





Results from Weisskopf-Ewing analysis

- Cross sections depend on the J^π distribution (WE limit not strictly valid)
- Largest uncertainties are below E_n=3 MeV and are due to J^π effects
- Deviations at higher energies are due to preequilibrium effects.

Results from Ratio analysis

- The cross sections show some dependence on J^π
- Agreement with expected cross section is very good (except for small energies and at 2nd-chance fission)
- Less J^π dependence and better agreement than for the Surrogate WE approach

Knowledge of J^π is important!

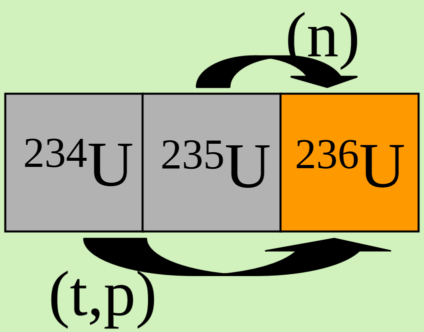
Knowledge of the CN J^π populations is important!

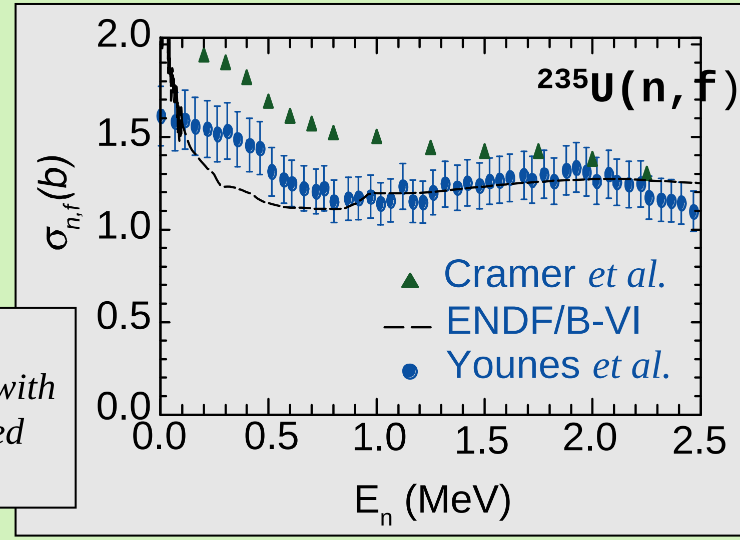
Younes and Britt

Phys. Rev. C **67** (2003) 024610, **68** (2003) 034610

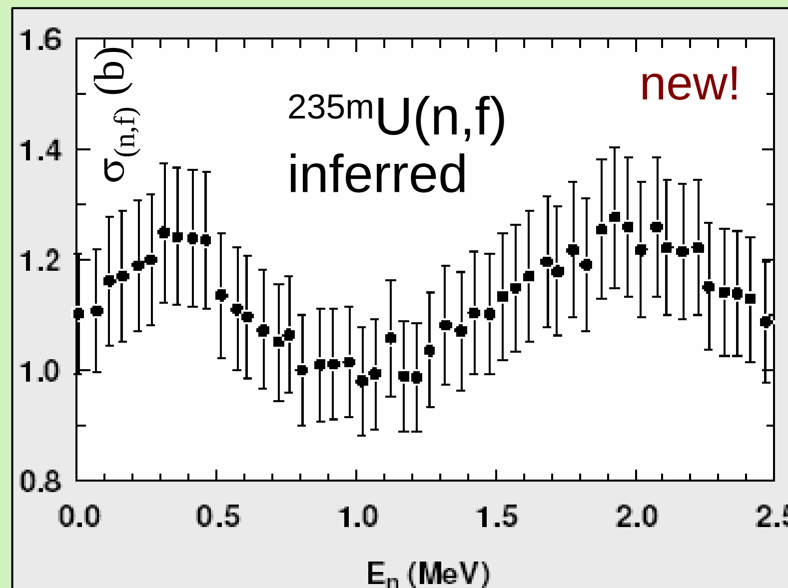
Re-analysis of (t,pf) data from the 1970s:

- **Incorporated effects of J^π population differences**
- Better optical model
- Fit model to experimental fission probabilities
- Added renormalization procedure to improve fit





Improved agreement with the evaluated result!



Need information on CN J^π populations

- To improve extracted cross sections
- To extend the method to lower energies
- To test validity of

III. Moving beyond current capabilities - R&D needs

Goals

- Achieve overall improvements of the Surrogate approach
- Extend the method to lower energies
- Extend the applications to other reaction mechanisms and isotopes (including unstable isotopes)
- Understand the limitations of the Surrogate approach
- Determine the reliability of the deduced cross sections and quantify uncertainties

Theory developments are needed to improve Surrogate approach…

1. **Predictions of spin-parity (J^{π}) distributions following a direct reaction**

Highly nontrivial, since it involves transfers and inelastic scattering to unbound states

2. **Quantitative description of the equilibration process of the intermediate nucleus following the direct reaction**

Challenging basic science: How does a highly-excited nucleus equilibrate?

- **How does the energy get distributed among all nucleons?**
- **What is the likelihood that particles are emitted prior to equilibrium? How does this change the J^{π} distribution?**

3. **Improved optical models (e.g., for extrapolations to unstable nuclei)**

4. **Improved level densities, strength functions, etc. (see D. Dean’s slide)**

Experimental developments are needed to improve Surrogate approach…

1. **Experiments that test theoretical predictions, e.g. experiments that provide information on CN J^{π} distributions (possibly from relative γ-ray intensities in γ-decaying CN).**

2. **Benchmark experiments that yield results which can be compared to known cross sections (-> L. Bernstein’s presentation)**

3. **Experiments that move into new territory (e.g. inverse kinematics with radioactive beams -> J. Cizewski’s presentation)**

4. **….**

IV. Synopsis

The Surrogate nuclear reaction approach is potentially very valuable for determining reaction cross sections of interest to AFC, SBSS, and astrophysics. It is the only indirect method for obtaining CN reaction cross sections.

Various approximations to the full Surrogate approach (Weisskopf-Ewing approximation, Surrogate Ratio method) show promising results for actinides.

To apply the method at lower energies, for other reaction mechanisms and in other regions of the nuclear chart, it becomes necessary to go beyond current approximations.

Theoretical and experimental R&D is needed to extend the applicability of the method to new regions (energy, isotopic chart, reaction mechanisms), to determine the reliability of the extracted cross sections and to quantify uncertainties.

There are very interesting basics physics problems associated with Surrogate reactions

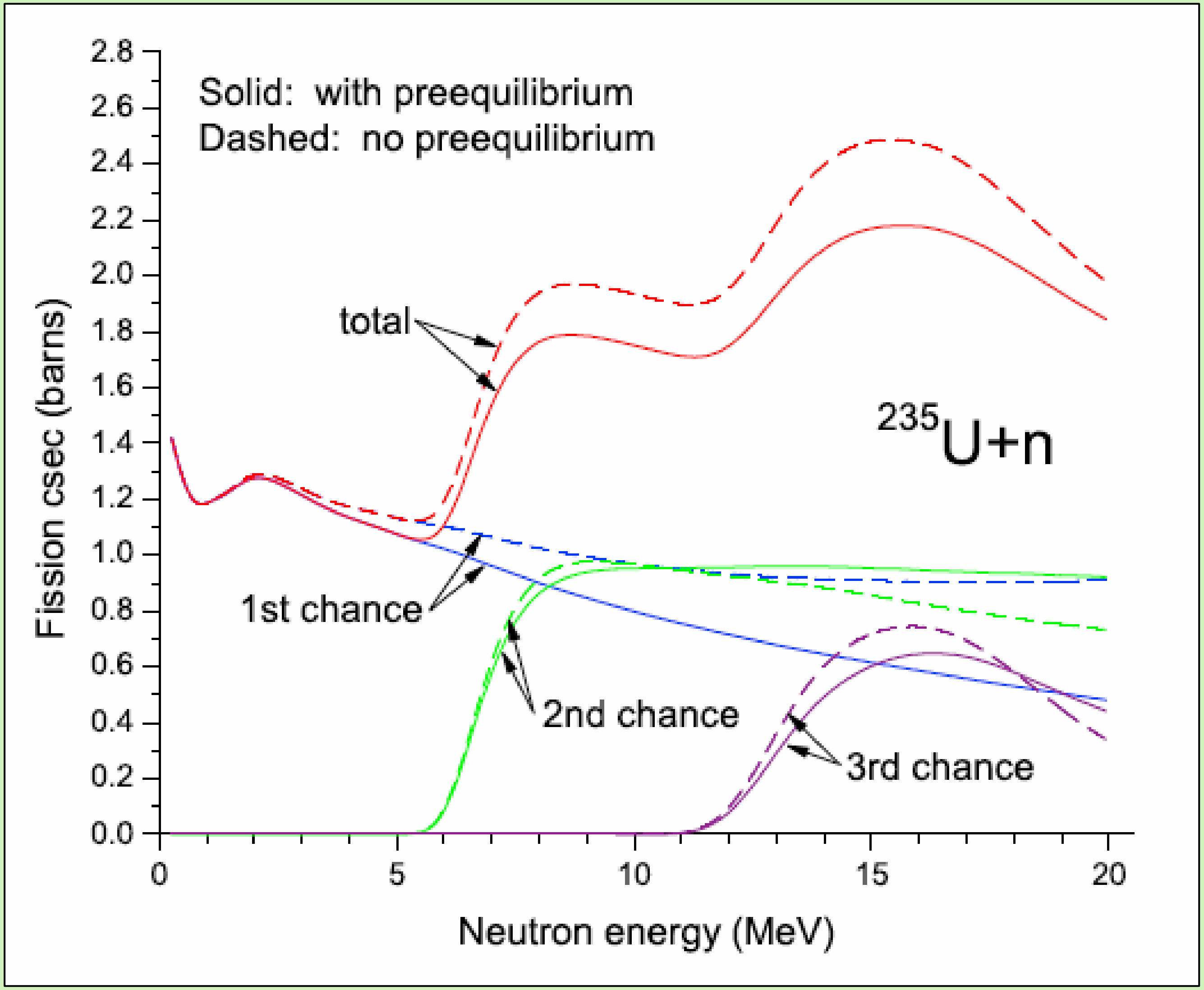
Collaborators

Theory:
F.S. Dietrich, V. Gueorguiev,
R. Hoffman, I. Thompson *(N Division, LLNL)*
C. Forssén (*Chalmers University)*

Experiment:
L. Ahle, J. Burke, L.A. Bernstein, J.A. Church
(N Division, LLNL)
D. Bleuel + *other experimentalists from LBNL*

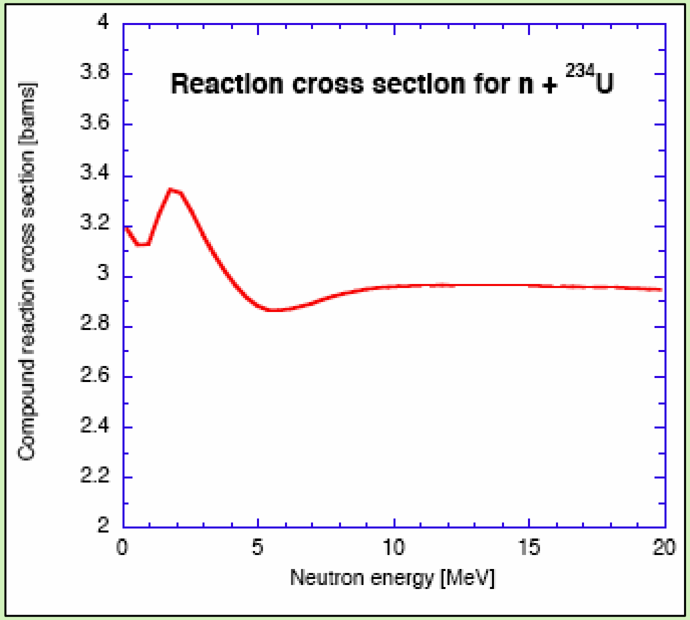
Appendix

Preequilibrium effects in the desired reaction

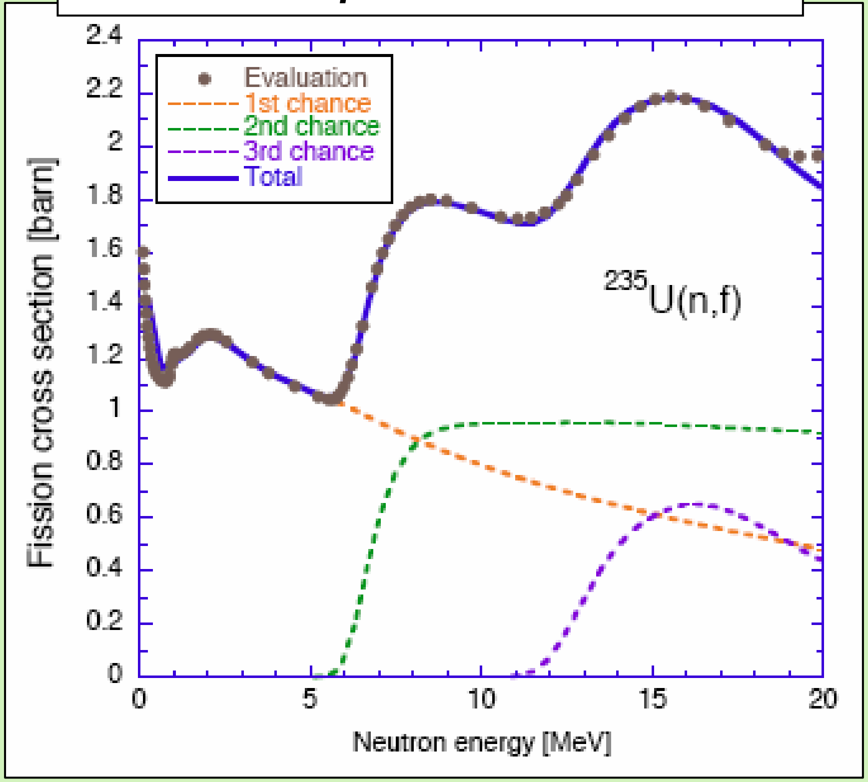


Details of the model

- Compound nuclei studied: ^{234}U and ^{236}U
- Level schemes and γ branchings from RIPL-2
- Level densities in Gilbert-Cameron form
- Deformed optical model (FLAP 2.2), neutron transmission coefficients independent of A



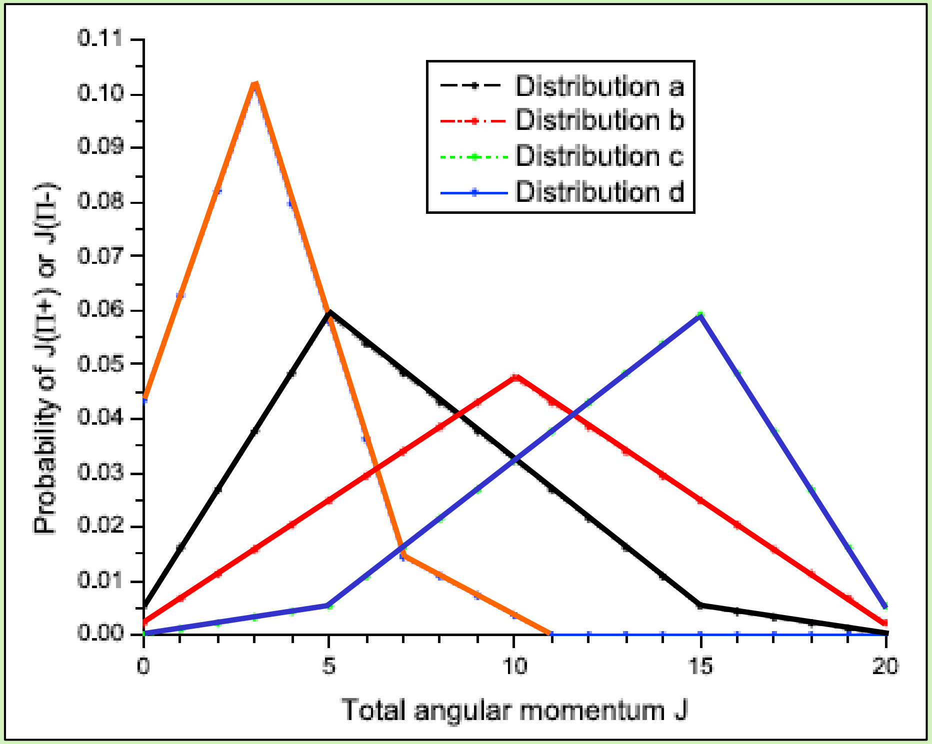
Fit to n + ^{235}U fission cross section



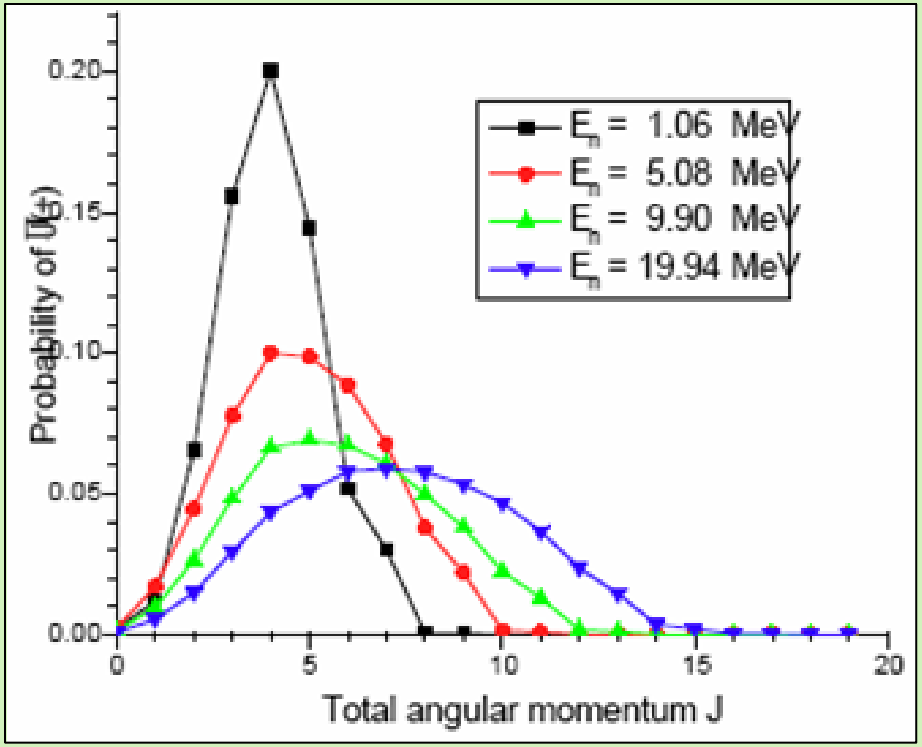
- Fission: 2-barrier model of Bjørnholm & Lynn; transition states represented by level density; barrier heights, curvatures, and level density parameters are fitted
- γ transmission coefficients calculated from Brink-Axel model, double-humped Lorentzian for giant dipole, small M1 component
- Width fluctuation corrections are not included

J^π populations of the decaying compound nucleus

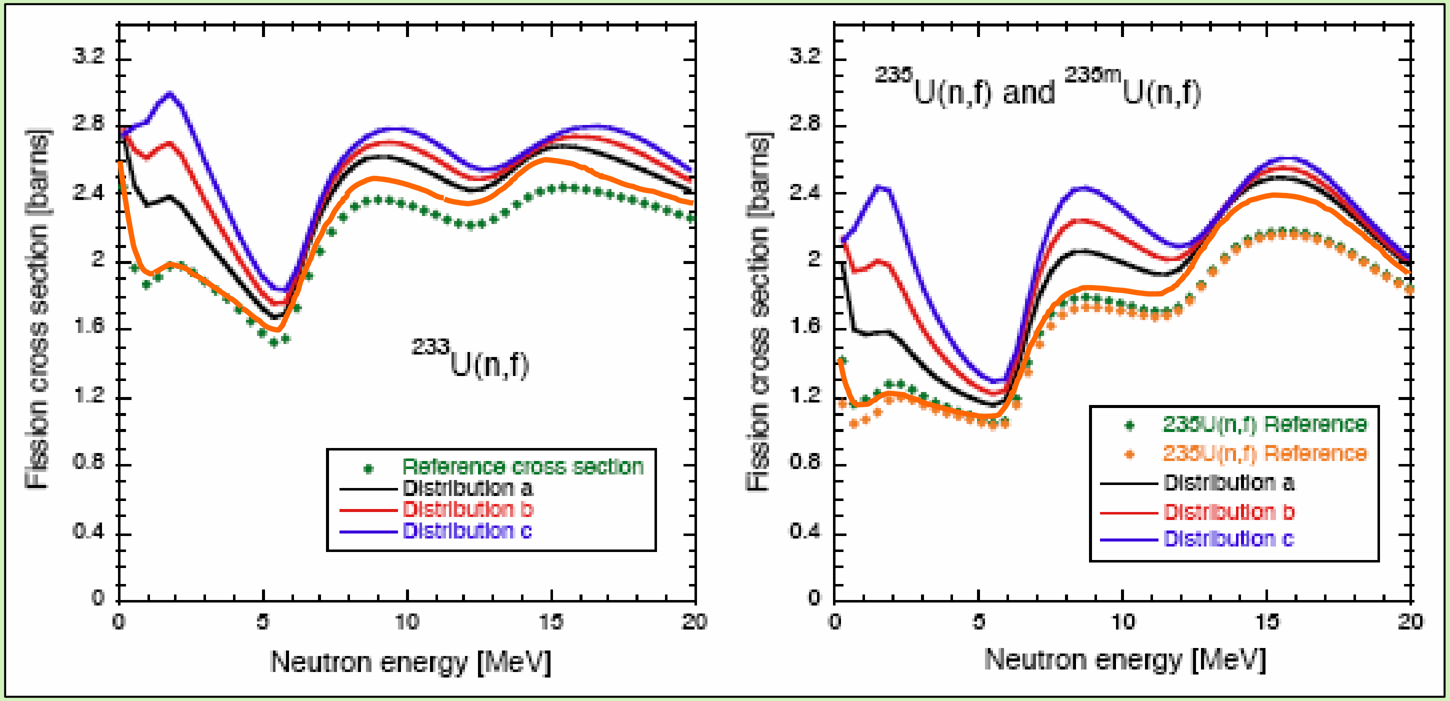
J^π populations considered in the simulations



J^π populations for n+^{235}U



(n,f) cross sections from a WE simulation



Observations

- The deduced cross sections are clearly dependent on the J^{π} distribution (WE limit not strictly valid)
- The largest uncertainty are below E_n=3 MeV and are due to angular-momentum effects
- Deviations at higher energies are due to preequilibrium effects.

- Identifying a Surrogate reaction that produces a CN similar to that of the desired reaction yields the best result for the extracted cross section
- The Surrogate reaction approach does not account for preequilibrium effects in desired reaction.